

What is claimed is:

Claims

- 1 1. A method of characterizing a mixture of components, the method comprising the
2 steps of:
 - 3 obtaining a plurality of spectrochromatograms of the mixture of components,
4 each of the spectrochromatograms being obtained under a respective one of
5 a plurality of different chromatographic conditions;
6 estimating the number of components and
7 performing component matching upon the spectrochromatograms using the
8 estimated number of components.
- 1 2. The method of claim 1 further comprising the step of determining each
2 component retention time in response to the component matching.
- 1 3. The method of claim 1 further comprising the step of determining each
2 component spectral shape in response to the component matching.
- 1 4. The method of claim 3 further comprising the step of using the component
2 spectral shape to identify the component.
- 1 5. The method of claim 1 further comprising the step of resolving at least one
2 component in the mixture of components.
- 1 6. A method of component peak matching comprising the steps of:
2 obtaining a plurality of spectrochromatographic data sets for a mixture of
3 components, each spectrochromatographic data set comprising
4 spectrochromatographic data;
5 creating an augmented spectrochromatographic data set by merging the
6 spectrochromatographic data sets into a matrix;
7 determining a preliminary estimate of the number of components (n) in the
8 augmented spectrochromatographic data set;
9 selecting the (n) most orthogonal spectrochromatographic data from the
10 augmented spectrochromatographic data set;
11 generating a refined key spectra set; and

12 determining the component retention times.

1 7. The method of claim 6 further comprising the step of:
2 validating each of the (n) most orthogonal spectrochromatographic data using
3 target factor analysis to generate the refined key spectra set.

1 8. The method of claim 6 further comprising the step of detecting missing
2 components using target testing of each spectrochromatographic data in the refined key
3 spectra set against each of the plurality of spectrochromatographic data sets.

1 9. The method of claim 6 wherein the step of determining a preliminary estimate
2 uses principle component analysis.

1 10. The method of claim 6 wherein the step of determining a preliminary estimate
2 uses single value decomposition.

1 11. The method of claim 6 wherein the step of determining a preliminary estimate
2 uses nonlinear iterative partial least squares.

1 12. The method of claim 6 wherein the step of selecting the (n) most orthogonal
2 spectra uses modified Iterative Key Set Factor Analysis.

1 13. The method of claim 6 wherein the step of determining the component retention
2 times comprises:
3 performing a regression using the refined key spectra set and the augmented data
4 matrix; and
5 determining retention times as maximum values.

1 14. A method for resolving a mixed sample of chromatographic components, the
2 method comprising the steps of:
3 selecting a plurality of differing chromatographic conditions;
4 performing a plurality of chromatographic runs on the mixed sample, each
5 respective run performed under a respective chromatographic condition;
6 obtaining spectrochromatographic data for the mixed sample during each of the
7 chromatographic runs;
8 creating an augmented data set from the spectrochromatographic data of the
9 plurality of chromatographic runs;

10 operating on the augmented data set to determine the retention times for each
11 component in the mixed sample; and
12 resolving each of the components.

1 15. The method of claim 14 further comprising the step of performing component
2 quantitation.

1 16. The method of claim 15 wherein the step of performing component
2 quantitation uses resolved spectra and concentration profiles.

1 17. The method of claim 14 further comprising the step of finding peak relative
2 areas using concentration profiles.

1 18. A method of obtaining the shape of components from spectrochromatographic
2 data comprising the steps of:
3 determining the number of components (n) and each component's retention time;
4 generating uniqueness vectors as initial estimates of spectrochromatographic
5 profiles; and
6 performing profile resolution on the spectrochromatographic data.

1 19. The method of claim 18 wherein the step of performing profile resolution uses
2 ALS MCR.